Amendments to the Claims:

This listing of claims will replace all prior versions and listings, of claims in the application:

Listing of Claims:

1.   *(Currently Amended)* A method of assessing a combinatorial library for complementarity to library a target having at least one binding site, said combinatorial library comprising a plurality of ligands, each based on a common core, said method comprising:

docking each ligand of the said plurality of ligands to the target molecule to generate a plurality of ligand positions relative to the target molecule in a plurality of ligand-target molecule complex formations, said plurality of ligand positions comprising a plurality of common core positions relative to the target molecule;

determining an rms deviation of each common core position of said plurality of common core positions from other common core positions; and

forming clusters according to said rms deviation.

2.   *(Previously Presented)* A method according to claim 1, additionally comprising rating complementarity of the combinatorial library to the target molecule according to number of ligands in a cluster having a minimum rms deviation relative to number of ligands in the combinatorial library.

3.   *(Original)* A method according to claim 1 wherein said determining an rms deviation comprises:

placing a grid around a binding site of the target molecule;

for each ligand position, determining a location on the grid corresponding to the center of mass of the common core; and

determining the rms deviation of each common core position from every other common core position having a location on the grid within a predetermined distance.

4.   *(Original)* A method according to claim 1 wherein said forming clusters comprises forming clusters using a single linkage clustering algorithm.

5.   *(Currently Amended)* A method according to claim 1 wherein said docking each ligand comprises:

performing a pre-docking conformational search to generate multiple solution conformations of each ligand;

generating a binding site image of the target molecule, said binding site image comprising multiple hot spots;

matching hot spots of the binding site image to atoms in at least one solution conformation of the multiple solution conformations of each ligand to obtain at least one ligand position relative to the target molecule in a ligand-target molecule complex formation; and

optimizing the at least one ligand position while allowing translation, orientation and rotatable bonds of the ligand to vary, and while holding the target molecule fixed.

6.   *(Currently Amended)* A system for assessing a combinatorial library for complementarily to a target having at least one binding site, said combinatorial library comprising a plurality of ligands, each based on a common core, said system comprising:

means for docking each ligand of the-said plurality of ligands to the target molecule to generate a plurality of ligand positions relative to the target molecule in a plurality of ligand-target molecule complex formations, said plurality of ligand positions comprising a plurality of common core positions relative to the target molecule;

means for determining an rms deviation of each common core position of said plurality of common core positions from other common core positions; and

means for forming clusters according to said rms deviation.

7.   *(Currently Amended)* A system according to claim 1according to claim 6, additionally comprising means for rating complementarity of the combinatorial library to the target molecule according to number of ligands in a cluster having a minimum rms deviation relative to number of ligands in the combinatorial library.

8.   *(Currently Amended)* A system according to claim 1according to claim 6 wherein said means for determining an rms deviation comprises:

means for placing a grid around a binding site of the target molecule;

means for, for each ligand position, determining a location on the grid corresponding to the center of mass of the common core; and

means for determining the rms deviation of each common core position from every other

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common core position having a location on the grid within a predetermined distance.

9.   *(Currently Amended)* A system ~~according-to-claim-1~~according to claim 6

wherein said means for forming clusters comprises means for forming clusters using a single linkage clustering algorithm.

10.   *(Currently Amended)* A system ~~according-to-claim-1~~according to claim 6

wherein said means for docking each ligand comprises:

   means for performing a pre-docking conformational search to generate multiple solution conformations of each ligand;

   means for generating a binding site image of the target molecule, said binding site image comprising multiple hot spots;

   means for matching hot spots of the binding site image to atoms in at least one solution conformation of the multiple solution conformations of each ligand to obtain at least one ligand position relative to the target molecule in a ligand-target molecule complex formation; and

   means for optimizing the at least one ligand position while allowing translation, orientation and rotatable bonds of the ligand to vary, and while holding the target molecule fixed.

11.   *(Currently Amended)* At least one program storage device readable by a machine, tangibly embodying at least one program of instructions executable by the machine to perform a method for assessing a combinatorial library for complementarity to a target having at least one binding site, said combinatorial library comprising a plurality of ligands, each based on a common core, said method comprising:

   docking each ligand of ~~the~~said plurality of ligands to the target molecule to generate a

plurality of ligand positions relative to the target molecule in a plurality of ligand-target molecule complex formations, said plurality of ligand positions comprising a plurality of common core positions relative to the target molecule;

   determining an rms deviation of each common core position of said plurality of common core positions from other common core positions; and

   forming clusters according to said rms deviation.

12.   *(Currently Amended)* The at least one program storage device ~~according-to claim-1~~according to claim 11, wherein said method additionally comprises rating

complementarity of the combinatorial library to the target molecule according to number of

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ligands in a cluster having a minimum rms deviation relative to number of ligands in the combinatorial library.

13.   *(Currently Amended)* The at least one program storage device ~~according to claim 1~~according to claim 11, wherein said determining an rms deviation comprises:

placing a grid around a binding site of the target molecule;

for each ligand position, determining a location on the grid corresponding to the center of mass of the common core; and

determining the rms deviation of each common core position from every other common core position having a location on the grid within a predetermined distance.

14.   *(Currently Amended)* The at least one program storage device ~~according to claim 1~~according to claim 11, wherein said forming clusters comprises forming clusters using a single linkage clustering algorithm.

15.   *(Currently Amended)* The at least one program storage device ~~according to claim 1~~according to claim 11, wherein said docking each ligand comprises:

performing a ~~pre-docking~~conformational search to generate multiple solution conformations of each ligand;

generating a binding site image of the target molecule, said binding site image comprising multiple hot spots;

matching hot spots of the binding site image to atoms in at least one solution conformation of the multiple solution conformations of each ligand to obtain at least one ligand position relative to the target molecule in a ligand-target molecule complex formation; and

optimizing the at least one ligand position while allowing translation, orientation and rotatable bonds of the ligand to vary, and while holding the target molecule fixed.